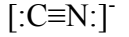
Formal Charges and Oxidation States

A. Formal Charges:

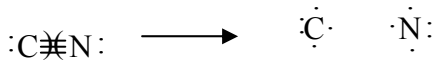
Formal charges in a molecule are determined by formal homolytic cleavage of all bonds. The charge of a resulting fragment is the formal charge of the corresponding atom in the molecule.

Example: the cyanide anion

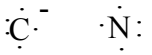
1. step: draw the Lewis structure of the molecule/molecular ion



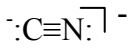
2. step: homolytically cleave all bonds (break all bonds right in the middle)



3. step: count the valence electrons of the fragments and compare that number with the number of valence electrons in the neutral atom (C atom: four valence electrons, N atom: five valence electrons). If the number of electrons in a fragment is less than that in the corresponding atom the fragment will be positively charged, if the number of electrons is larger the fragment will be negatively charged.



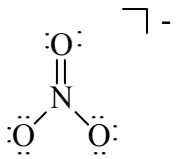
4. step: write the formal charges into the Lewis structure, as + or 2+ or -, etc. Alternatively you can write formal charges with circling the sign, for example ⊕ or 2⊕.



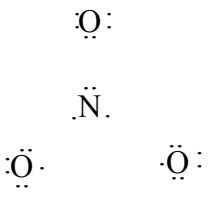
You should always indicate the formal charges in Lewis structures! The sum of the formal charges is equal to the total charge of the molecule. If the formal charges are determined correctly, the sum will show you if you included the correct number of electrons in the Lewis structure.

Example:

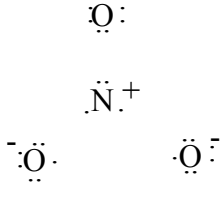
1. Lewis structure



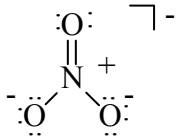
2. Homolytic bond cleavage



3. Charges of fragments



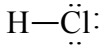
3. Indicating formal charges in Lewis structure



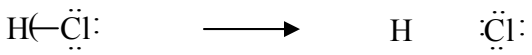
B. Oxidation states:

Oxidation states of atoms in convalent compounds are determined by formally cleaving every bond heterolytically in such a way that the bonding electron pair (or bonding electron pairs for multiple bonds) will remained at the more electronegative element. The charges of the resulting fragments are the oxidation states of those atoms in the compounds.

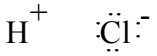
1. step: draw Lewis structure



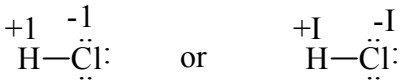
2. step: cleave bonds heterolytically considering electronegativity



3. step: determine the charge of every fragment by comparing the number of electrons in the fragment to that in the neutral atom.



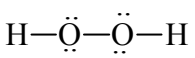
4. step: indicate the oxidation states in your Lewis structure. Oxidation states are denoted as + or – followed by the number in Arabic or Roman numerals: +5 or +V



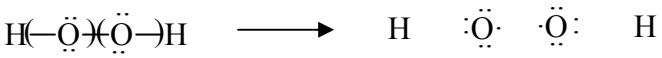
- Include the oxidation states of the atoms in a Lewis structure only if you are asked to do so.
- In the case of homonuclear bonds (bonds between atoms of the same element) the bond will be cleaved homolytically (since the electronegativity difference is zero).
- The sum of the oxidation states will be equal to the overall charge of the molecule.

Example: H-O-O-H

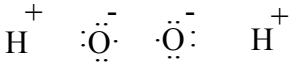
1.step: Lewis structure



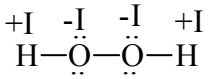
2.step: Formal bond cleavage



3. step: Charges of fragments



4. step: Indicate oxidation states in Lewis structure



- In the case of monoatomic ions (Na^+ or Cl^-) the charge of the ion is the oxidations state.